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KINETIC CHARACTERISTICS OF IGNITION DISPERSED CONDENSED SUBSTANCE SINGLE HEATED TO A HIGH TEMPERATURE OF THE PARTICLES

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Abstract. Kinetic parameters of ignition are defined by the results of performed experimental and theoretical investigations of regularities of the process ignition dispersed solid condensed substance when interacting with a high-temperature metal particles.

1 Introduction

The use of traditional solid fuels, such as low-calorie coal, is one of the actual directions of development heat power engineering [1]. Any condensed substance (CS) in particulate (dispersed) state burn up in the furnaces of steam boilers more efficiently [2]. If there is some grinding mechanoactivation substances [2], which resulted in the change process performance termokinetics ignition and subsequent burning fuels. Interaction shredded combustible materials with “hot” particles formed as a result of friction or shock, characterized by a high risk of transport and storage of such fuels [3]. Well researched conditions and ignition characteristics of a large group uncomminuted condensed substances (HF), for example, composite solid propellants [4-6], forest fuels [7,8], liquid fuels [9,10] local energy sources. Well researched conditions and ignition characteristics of a large group uncomminuted condensed substances (CS), for example, composite solid propellants [4-6], combustible forest materials [7,8], liquid fuels [9,10] local energy sources. Regularities of ignition dispersed CS studied to a much lesser extent [11].

Results [3-10] and theoretical investigation [12-14] can not be directly used to predict the conditions and the ignition characteristics of crushed solid fuels. On the example of wood sawdust [11] established significant differences in the mechanisms of heat transfer layer dispersed CS and monolithic condensed matter. Therefore, the kinetic characteristics of the ignition processes in these two cases may differ materially. Therefore to present day is no information about these characteristics the even for prevalent used in the heat-and-power engineering of solid fuels.

The purpose of this work is determination of thermochemical characteristics (activation energy and pre-exponential factor) for reaction of gas-phase dispersed condensed substance ignition (coal dust) according to experimental studies results.

2 Experimental technique

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The experimental investigations of ignition for solid CS by the single steel particle warmed to high temperatures was held used the plant according the methods [5]. Analysis and generalization of experimental data [3, 5, 7,8] on dependence of ignition delay time on initial temperature of heating source allow formulating an important statement regulating experimental conditions for determination of kinetic parameters. It is reasonable to conduct an experiment at the maximum possible initial temperature (T_p) of the particle (source of energy) for ensuring minimal errors of ignition delay time (t_{ign}) measurements.

The results of experiments performed with the dispersed coal in the form of relation $t_{ign}=f(T_p)$ are shown in Fig. The experimental results are shown in Fig. 1. The kinetic parameter values of ignition reaction – E_1 (activation energy) and the product $Q_0k_1^0$ (product of the thermal effect of the reaction on the preexponential factor) were calculated by the expression [15]:

$$t_{ign} = 1,18 \left(1 - \frac{T_0}{T_p} \right) \sqrt{T_p - T_0} \frac{C}{Q_0 k_1^0} \sqrt{\frac{E_1}{R_t}} \exp \left(\frac{E_1}{R_t T_p} \right). \quad (1)$$

Nomenclature were accepted: t_{ign} – ignition delay time, sec; T_0 – initial temperature of air and CS, K; T_p – initial temperature of “hot” particle, K; C – specific heat, J/(kg·K); Q_0 – thermal effect of oxidation reaction, J/kg; k_1^0 – preexponential factors, s⁻¹; E_1 – activation energy of oxidation reaction, J/mol; R_t – absolute gas constant, J/(mol·K).

Two points of the experimental curve (Fig., curve 1) were used for calculating of two unknowns. The points make a connection between T_p and t_{ign} in area of relatively high initial temperatures of energy source. Thus it is sufficiently to solve a system of two transcendental equations for determination the kinetic parameters.

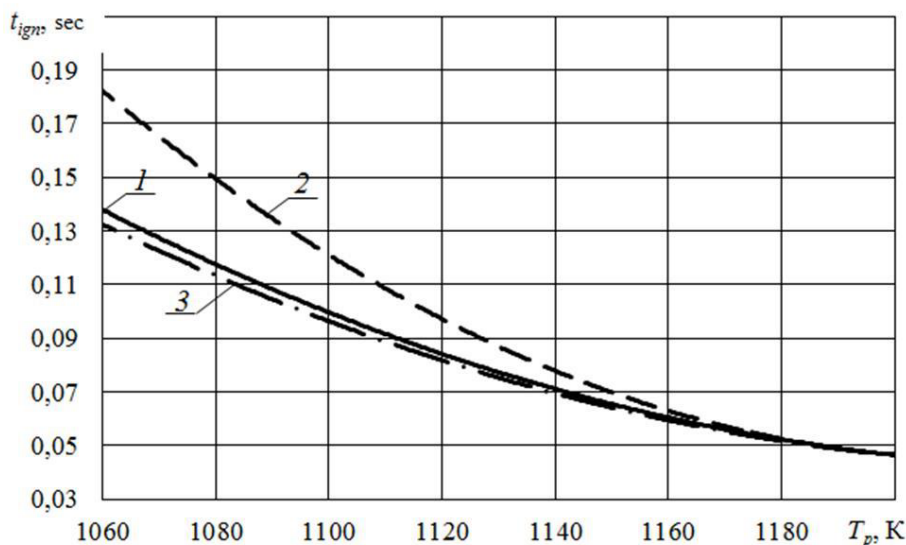


Figure 1. The dependence of the ignition delay time t_d on the initial temperature T_p of “hot” particle: 1 – experimental curve, 2 – theoretical curve at $Q_0 k_1^0 = \text{const}$, 3 – theoretical curve at $Q_0 k_1^0 = f(T_p)$.

The kinetic parameters values of the oxidation reaction were calculated for the variation range of the hot particle initial temperature from 1050 K to 1200 K: $E_1 = 84 \cdot 10^3$ J/mol, $Q_0 k_1^0 = 5,516 \cdot 10^{11}$ J/(kg·s).

The verification of the findings characteristics of the ignition process. Toward this end we solve the problem in describing the process under study the mathematical model [13,14] developed for the heating conditions of liquid fuels “hot” particles.

3 Mathematical model

Mathematical modeling of physical and chemical processes taking place during the ignition has been realized in system “dispersed CS – energy source with limited heat content– air”. It was assumed that the local energy source – the small-size ($r_p=r_1=3\cdot 10^{-3}$ m, $h_p=z_2-z_1=3\cdot 10^{-3}$ m) disk-shaped steel particle heated to high temperature is deposited on the surface of the dispersed coal.

The objective of this analysis is to assessment of reliability of the determined values of the kinetic ignition parameters by means of Arrhenius dependence (Fig. 1, curve 1) of the rate of oxidation reaction on the local energy source’s initial temperature.

The following complex of ignition criteria was used which allows considering that specific features of the heat-and-mass transfer processes in the system with the local power source during the induction period:

1. Energy released by the oxidation reaction of the gaseous products of thermal decomposition of dispersed CS’s particles is greater than heat transferred from the heating source to the reaction zone.

2. The gas mixture temperature is greater than the initial temperature of the hot particle in the reaction zone of intensive oxidation.

The ignition problem has been solved in an axially symmetric formulation in a cylindrical coordinate system with the origin coincident with the symmetry axis of the hot particle. The given below system of nonlinear non-stationary differential equations describes a complex of the heat and mass transfer processes with the phase transformations and chemical reactions at $0 < t < t_d$.

The energy equation for the gas mixture of oxidant (air) with gas components of porous CS particles thermal decomposition ($r_1 < r < r_l$, $z_1 < z < z_2$; $0 < r < r_l$, $z_2 < z < z_h$):

$$\rho_1 C_1 \frac{\partial T_1}{\partial t} = \lambda_1 \left(\frac{\partial^2 T_1}{\partial r^2} + \frac{1}{r} \frac{\partial T_1}{\partial r} + \frac{\partial^2 T_1}{\partial z^2} \right) + Q_o W_o, \quad (2)$$

where $W_o = \rho_1 C_o^1 C_f^1 k_1^0 \exp\left(-\frac{E_1}{R_l T_1}\right)$ is mass rate of combustible gases oxidation in the air [15].

The heat transfer equation for the metallic particle ($0 < r < r_l$, $z_1 < z < z_2$):

$$\rho_2 C_2 \frac{\partial T_2}{\partial t} = \lambda_2 \left(\frac{\partial^2 T_2}{\partial r^2} + \frac{1}{r} \frac{\partial T_2}{\partial r} + \frac{\partial^2 T_2}{\partial z^2} \right). \quad (3)$$

The energy equation for porous CS ($0 < r < r_l$, $0 < z < z_1$):

$$\rho_3 C_3 \frac{\partial T_3}{\partial t} = \lambda_3 \left(\frac{\partial^2 T_3}{\partial r^2} + \frac{1}{r} \frac{\partial T_3}{\partial r} + \frac{\partial^2 T_3}{\partial z^2} \right) + Q_3 W_3, \quad (4)$$

where $W_3 = \varphi_3 \rho_3 k_3^0 \exp\left(-\frac{E_3}{R_l T_3}\right)$ is mass rate of porous CS particles thermal decomposition [15].

The diffusion equation for the combustible gases in the oxidant (air) ($r_1 < r < r_l$, $z_1 < z < z_2$; $0 < r < r_l$, $z_2 < z < z_h$):

$$\rho_f^1 \frac{\partial C_f^1}{\partial t} = \rho_f^1 D_f^1 \left(\frac{\partial^2 C_f^1}{\partial r^2} + \frac{1}{r} \frac{\partial C_f^1}{\partial r} + \frac{\partial^2 C_f^1}{\partial z^2} \right) - W_o. \quad (5)$$

The balance equation for the gas mixture ($r_l < r < r_l$, $z_1 < z < z_2$; $0 < r < r_l$, $z_2 < z < z_h$)

$$C_f^1 + C_o^1 = 1.$$

Nomenclature were accepted: r, z – coordinates of the rectangular system, m; r_l, z_h – solution domain extent, m; λ – thermal conductivity, W/(m·K); ρ is density, kg/m³; Q_3 – thermal effect of gasification reaction, J/kg; k_3^0 – preexponential factors, s⁻¹; E_3 – activation energy of gasification reaction, J/mol; C_f^1 – dimensionless mass concentration of combustible gases in the gas mixture ($0 < C_f^1 < 1$), C_o^1 – dimensionless mass concentration of oxidant (air) in the gas mixture; subscripts “1”, “2”, “3” correspond to gas mixture, steel particle, dispersed condensed substance.

Initial conditions at $t=0$:

$$\begin{aligned} T_1 &= T_0, C_f^1 = 0; r_l < r < r_l, z_1 < z < z_2; 0 < r < r_l, z_2 < z < z_h; \\ T_2 &= T_p, 0 < r < r_l, z_1 < z < z_2; \\ T_3 &= T_0, \varphi_f^3 = \varphi_f^{30}; 0 < r < r_l, 0 < z < z_1. \end{aligned} \quad (7)$$

Boundary conditions at $0 < t < t_d$:

1. On symmetry axis and external borders we set for all equations the condition of gradients vanishing of corresponding functions:

$$r=0, 0 < z < z_1; r=r_l, 0 < z < z_1: \frac{\partial T_3}{\partial r} = 0; \quad (8)$$

$$r=0, z_1 < z < z_2: \frac{\partial T_2}{\partial r} = 0; \quad (9)$$

$$r=0, z_2 < z < z_h: \frac{\partial T_1}{\partial r} = 0, \frac{\partial C_f^1}{\partial r} = 0; \quad (10)$$

$$r=r_l, z_1 < z < z_h: \frac{\partial T_1}{\partial r} = 0, \frac{\partial C_f^1}{\partial r} = 0; \quad (11)$$

$$z=0, 0 < r < r_l: \frac{\partial T_3}{\partial z} = 0; \quad (12)$$

$$z=z_h, 0 < r < r_l: \frac{\partial T_1}{\partial z} = 0; \frac{\partial C_f^1}{\partial z} = 0. \quad (13)$$

2. Thermal interaction between system components was described by boundary condition of type IV with allowance for finely grinded coal particles gasification on the site of a surface closed by “hot” metallic particle:

$$r=r_l, z_1 < z < z_2: -\lambda_2 \frac{\partial T_2}{\partial r} = -\lambda_1 \frac{\partial T_1}{\partial r}, T_2 = T_1, \frac{\partial C_f^1}{\partial r} = 0; \quad (14)$$

$$z=z_2, 0 < r < r_l: -\lambda_2 \frac{\partial T_2}{\partial z} = -\lambda_1 \frac{\partial T_1}{\partial z}, T_2 = T_1, \frac{\partial C_f^1}{\partial z} = 0; \quad (15)$$

$$z=z_1, 0 < r < r_l: -\lambda_3 \frac{\partial T_3}{\partial z} = -\lambda_2 \frac{\partial T_2}{\partial z}, T_3 = T_2, \frac{\partial C_f^1}{\partial z} = 0; \quad (16)$$

$$z=z_1, r_l < r < r_l: -\lambda_3 \frac{\partial T_3}{\partial z} = -\lambda_1 \frac{\partial T_1}{\partial z}, T_3 = T_1, -\rho_1 D_f^1 \frac{\partial C_f^1}{\partial z} = W_g, \quad (17)$$

$$\text{где } W_g = \int_{z=0}^{z=z_1} \varphi_3 \rho_3 k_3^0 \exp\left(-\frac{E_3}{R_l T_3}\right) dz. \quad (18)$$

Gasification rate of dispersed CS particles on the surface closed by a “hot” particle was defined by a ratio:

$$z=z_1, 0 < r < r_l: W_{g\Sigma} = \int_{r=0}^{r=r_l} W_g(r) dr. \quad (19)$$

Total gas-arrival $W_{g\Sigma}$ was distributed in a small vicinity of a particle according to expression:

$$z=z_1, r_l < r < r_l + 10h_r: W_g^S(r)_k = W_g(r)_k + \frac{1,1-0,1k}{10} W_{g\Sigma}, k = 1; 2; \dots; 10, \quad (20)$$

where $W_g(r)_k$ is mass rate of gasification on k^{th} step along an axis r without additional gas-arrival from the site of a surface closed by a “hot” particle;

$W_g^S(r)_k$ is total gasification rate on k^{th} step along an axis r in a vicinity of a “hot” particle.

The set of nonlinear non-stationary differential equations in private derivatives (2)–(6) with the corresponding initial and boundary conditions was solved by the method of final differences with use of algorithms [9,10].

4 Results and discussion

The numerical investigation was carried out for the following values of parameters: CS and air initial temperature $T_0=300$ K, steel particle initial temperature $T_p=1050\div 1200$ K; volume fraction of a substance capable of chemical reaction $\varphi_3=0.5$; kinetic parameters of the thermal decomposition reaction of CS – $E_3=195\cdot 10^3$ J/mol, $Q_3k_3^0=25.5\cdot 10^{14}$ J/(kg·s); kinetic parameters of the oxidation reaction of the gas mixture were calculated by the experimental dependence $t_{ign}=f(T_p)$:

$$E_1=84\cdot 10^3 \text{ J/mol}, Q_0k_1^0=5.516\cdot 10^{11} \text{ J/(kg}\cdot\text{s)}.$$

Thermophysical characteristics of substances are listed below:

$$\lambda_o^1=0.026 \text{ W/(m}\cdot\text{K)}; \rho_o^1=1.161 \text{ kg/m}^3; C_o^1=1190 \text{ J/(kg}\cdot\text{K)};$$

$$\lambda_2=49 \text{ W/(m}\cdot\text{K)}; \rho_2=7831 \text{ kg/m}^3; C_2=470 \text{ J/(kg}\cdot\text{K)};$$

$$\lambda_f^1=0.072 \text{ W/(m}\cdot\text{K)}; \rho_f^1=2.378 \text{ kg/m}^3; C_f^1=3876 \text{ J/(kg}\cdot\text{K)};$$

$$\lambda_f^3=0.186 \text{ W/(m}\cdot\text{K)}; \rho_f^3=1400 \text{ kg/m}^3; C_f^3=1310 \text{ J/(kg}\cdot\text{K)}.$$

Has been found (Fig. 1) that the experimental (curve 1) and calculated (curve 2) as a result of solving the problem (2)–(20) values of t_{ign} (for identical temperatures) differ nearly by 25 % providing by relatively low values of T_p . The reasons for rejection t_{ign} , can be explained by the features of gas-phase ignition with local heating of substance as well as by the specificity of heat and mass transfer in the heated layer of dispersed solid fuel.

For a formal description of the ignition process the analysis of received experimental data has been executed considering a possible dependence between the pre-exponential factor and temperature. The following approximation expression was received:

$$Q_0k_1^0=(2,193\cdot 10^6-2,493\cdot 10^3\cdot T_p+0,987\cdot T_p^2) \text{ Дж/(кг}\cdot\text{с)}, \text{ при } T_p=1050\div 1200 \text{ K.} \quad (21)$$

The Fig. shows the theoretical dependence $t_{ign}=f(T_p)$ – curve 3 obtained by numerical simulation of the ignition process using the approximated expression (21). An acceptable agreement between the experimental and calculated values of the ignition delay times at low temperatures is can be noted. The extreme deviations of the t_{ign} represent less than 3.5% that does not exceed the error of the experimental values t_{ign} . The type of the approximation dependence (21) allows to suggest that the model (1) gives a very good description of the actual process due to some “redundancy” of heat entering to the reaction zone. The heat transfer conditions in the case of dispersed substance as well as for the mixture of fuel and oxidant have a little effect on the chemical reaction rate if T_p is greater than some limiting value (in that case $T_p\approx 1180$ K). At relatively low temperature of local source the conditions of energy supply to the zone of intensive interactions have a prior importance. Summarizing the results of the research it can be concluded that we can always choose such variation range of the initial temperature of the heat source where the kinetics of the ignition process can be

determined by the formula (1) [15] with high accuracy for the ignition of dispersed CS at local heating conditions. At low T_p is necessary to consider the effect of temperature on the kinetic constants.

5 Conclusions

Investigation results allow making a conclusion about the possibility to determine the kinetic characteristics of the gas-phase ignition of dispersed CS by a local source at high temperatures using relatively simple approach developed long ago [15].

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